Supplement of

Diurnal simulations on atmosphere-snow water vapor exchange and the associated isotope effects at Dome Argus, Antarctica

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Table S1. List of variables in the model

Variables	Description (Unit)
E_x	Air-snow exchange flux ($kg \cdot m^{-2} \cdot s^{-1}$)
LE	Latent heat ($W \cdot m^{-2}$)
ρ_v	Dry air density ($kg \cdot m^{-3}$)
T_a	Air temperature at 4m height (K)
P_a	Atmospheric pressure (hPa)
L_s	Sublimation heat constant ($J \cdot kg^{-1}$), $L_s = 2.86 \times 10^6$ $J \cdot kg^{-1}$
z	Reference height in the boundary layer (m), z = 4m
r_a	Aerodynamic resistance from a reference height in the boundary layer to snow surface ($s \cdot m^{-1}$)
q_s	Saturated specific humidity over ice surface derived from the Clapeyon-Clausius equation ($kg \cdot kg^{-1}$)
RH_i	Calibrated relative humidity over ice surface (%)
q_a	Specific humidity over ice surface ($kg \cdot kg^{-1}$)
$dq_a/dt \times dT/dt$	Time derivatives of specific humidity and air temperature
C_E	Transfer coefficient for humidity
u_z	Wind speed ($m \cdot s^{-1}$)
k	von-karman constant, k=0.40
z_0	Surface roughness length for humidity exchange (m), $z_0=2.44 \times 10^{-4}$ m at Dome A
Ψ_M	Diabatic corrections with respect to the ratio of the reference layer height
L	Monin-Obukhov length (m)
$\bar{\theta}$	Mean potential temperature between the surface and a reference height in the boundary layer (K)
θ	potential temperature at the snow surface (K)
θ_z	potential temperature at the reference height (K)
u*	Friction velocity ($m \cdot s^{-1}$)
θ*	Temperature turbulent scale (K)
g	Gravity acceleration ($m \cdot s^{-2}$), g=9.8 m/s^2
Ri	Richardson number
M_s	Snow mass (kg)
M_v	Water vapor mass (kg)
ρ_s	Snow density ($kg \cdot m^{-3}$)
h_0	Snow height at initial time (m)
H_0	Near-surface boundary height at initial time (m)
R_s	Ratio between the abundance of heavy isotopes (^{18}O and D) and light isotopes (^{16}O and H) in the snow reservoir
R_v	Ratio between the abundance of heavy isotopes (^{18}O and D) and light isotopes (^{16}O and H) in the atmospheric water vapor reservoir
R_{Ex}	Ratio between the abundance of heavy isotopes (^{18}O and D) and light isotopes (^{16}O and H) in air-snow vapor exchange flux
δ	Another denotation of isotopic ratio (‰)
δS_0	Snow isotopic composition at initial time (‰)
δV_0	Water vapor isotopic composition at initial time (‰)
k'	Diffusion coefficient
α_f	Efficient fractionation coefficient
α_e	Equilibrium fractionation coefficient
α_k	Kinetic fractionation coefficient
$D_i/D_{i'}$	Ratio between the molecular diffusivity of major and minor water isotopic species in air
σ	Stefan–Boltzmann constant ($W \cdot m^{-2} \cdot K^{-4}$), $\sigma = 5.67 \times 10^{-8}$ $W \cdot m^{-2} \cdot K^{-4}$
ϵ	snow emissivity, $\epsilon = 0.93$
LW_{dn}	downward longwave radiative fluxes ($W \cdot m^{-2}$)
LW_{up}	upward longwave radiative fluxes ($W \cdot m^{-2}$)

Texts S1. Meteorological data processing

At Dome A, air temperature measured at all 3 heights exhibits a harmonic on the diurnal scale. An interpolation method is thus presented to make a continuous record of air temperature when observations are missed (e.g., Laepple et al., 2018). The formula used is as follows:

$$T_a=T_{mean}+A1\cos(\omega t+\Phi)+A2\sin(\omega t+\Phi) \quad (S1)$$

where T_{mean} denotes the daily mean from temperature observations, A1 and A2 are the amplitude of the harmonics, ω and t is the angular frequency and time, Φ denotes the phase of first harmonics.

The observed relative humidity (RH_w) at height z are normalized to the saturation vapor pressure at the surface temperature. Then they requires previously calibration when it acts as the super-saturation coefficient for calculating the kinetic fractionation factor in the model (Eq.15). However, the common correction method developed by Anderson (1994) fails to capture the super-saturation conditions at temperature < -20°C when the AWS probe is affected by frost deposition (Makkonen, 1996; 2005). To solve the issue, we proposed an improvement method, based on the calibration procedures of Anderson (1994), to rescale RH at Dome A. The details are follows: 1) RH_w observations were converted to RH_I^0 using Eq. S2, 2) The RH_I^0 were calibrated using the ideal maximum RH_I at each air temperature point ($RH_I^1 = RH_I^0/ RH_I^{max}$). Note the RH_I^{max} was set to the 95th percentile of RH_I^0 at each air temperature point, 3) For RH_I^1>100% (i.e., super-saturation condition), RH_I^1 was multiplied by a factor to calculate RH as the final result. This factor was the ratio of saturation vapor pressure over ice at the ambient air temperature. The rising amplitude of the temperature was depended on comparisons of atmospheric moisture measurements between AWS and frost-point hygrometer at Dome C (Genthon et al., 2017).

$$RH_i = (q_s^w/q_s^i)*RH_w \quad (S2)$$

Texts S2. Uncertainty analysis

At each time step, we firstly calculated the uncertainties of wind speed (Q_U), air temperature (Q_{T4m}), relative humidity (Q_{RH}) using the hourly AWS observations of those selected days for each parameter. The same method was also used to estimate the variablity in surface temperature calculations (Q_{Ts}). Then the variations of the error of friction velocity (Q_{u*}), aerodynamic resistance (Q_{ra}), latent heat (Q_{LE}) and specific humidity (Q_q) were estimated through the error propagation method for a multi-variable function (e.g., Radic et al., 2017). The uncertainties for those meteorological parameters can thus be propagated into the final error for u*, r_a, LE and q.

Based on uncertainty analysis of u*, r_a and q, we used a Monte Carlo approach to quantify uncertainties in the modeled vapor exchange flux (E_x). This approach is model running 1000 times with randomly perturbed values of u*, r_a and q. For each Monte Carlo run, we picked the values of perturbed parameters assuming a normal distribution of mean values and standard deviations. Then the errors of E_x can be presented by a standard deviation of 1000 ensemble runs and labeled as Q_{ra}', Q_{u*}'and Q_q'. Finally, the total error of E_x was assessed as the root mean sum of these three individual estimations. The MATLAB code of uncertainty propagation functions are sourced from https://www.mathworks.com/matlabcentral/fileexchange/89812-uncertainty-propagation-functions (Joe Klebba, 2022).

The same Monte Carlo method were also used to quantify the uncertainties (Q_δ)

in isotopic values, but with uncertainties of E_x and effective fractionation coefficient (α_f). Note that the uncertainties of effective fractionation coefficient (α_f) were estimated using error propagation method and observed temperature data.

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